

AITHYRA

Collaboration AITHYRA and Technical University of Vienna

Michael Bronstein, AITHYRA Scientific Director AI and Honorary Professor of the Technical University of Vienna in collaboration with Ismail Ilkan Ceylan, expert in graph machine learning, invites outstanding candidates to apply for a postdoctoral research position in **Geometric Deep Learning**, with a strong emphasis on applications to biology and scientific discovery. This unique research collaboration between **AITHYRA and the Technical University of Vienna** offers an exceptional opportunity to engage in both **foundational machine learning research** and **high-impact interdisciplinary applications** in the natural sciences. The position offers access to top-tier academic and industry research ecosystems and is ideally suited for researchers seeking to push the boundaries of geometric and graph-based learning in real-world scientific contexts. The research program is flexible and interdisciplinary.

Postdoctoral Researcher Position in Geometric Deep Learning & AI for Science (f/m/d)

AITHYRA, the place where magic happens!

The mission of AITHYRA, the new Research Institute of Biomedical Artificial Intelligence of the Austrian Academy of Sciences in Vienna is to transform the way life sciences are conducted using AI to drive the biological revolution in the next decade, with the ultimate goal of improving human health.

<https://www.oeaw.ac.at/aithyra>

TU Wien, where we dare to reason!

The Technical University of Vienna - TU Wien covers a wide spectrum of scientific concepts from abstract pure research and the fundamental principles of science to applied technological research and partnership with industry. The TU Wien is Austria's largest research and educational institution in the field of technology and natural sciences. <https://www.tuwien.at/en>

Your Tasks, Core Themes

Candidates will have the opportunity to pursue one or more of the following core themes:

1. Large Pre-Trained Models for Multi-Modal Reasoning

This project explores the integration of graph-based foundation models (e.g., knowledge graphs) with large language models (LLMs) to build AI systems capable of reasoning across diverse scientific data modalities such as structured databases, ontologies, and unstructured text. The goal is to enable automated hypothesis generation and obtain scientific insights, with potential applications in biomedical discovery, literature mining, and cross-domain reasoning.

2. Deep Surrogate Models for Complex Scientific Systems

This theme focuses on building deep learning-based surrogate models that approximate complex physical and biological systems traditionally modeled by PDEs or other computationally expensive simulations. By incorporating physical priors such as conservation laws and symmetries into architectures like neural operators, physics-informed neural networks (PINNs), and graph-based solvers, the project aims to accelerate simulations in areas including protein folding, gene regulation, drug–target interactions, and multi-scale biomedical modeling.

3. Deep Learning on Graphs with Higher-Order Structures

This project develops neural architectures capable of modeling higher-order relational structures such as hypergraphs and simplicial complexes, which are prevalent in complex biological systems like protein assemblies, signaling pathways, and metabolic networks. The goal is to build foundation models capable of learning from richly structured or semi-structured data where traditional graph neural networks may fall short, enabling better representation, inference, and discovery in complex domains.

4. Theoretical Foundations of Geometric Deep Learning

This theme addresses foundational questions in geometric deep learning, including the expressiveness of graph neural networks under symmetry constraints, their optimization dynamics, and their generalization behavior—particularly in low-data or out-of-distribution settings. The work combines formal theoretical analysis with practically motivated case studies, offering a strong foundation for researchers interested in advancing the mathematical understanding of geometric deep learning.

Your Qualifications

- **PhD** (or near completion) in computer science, machine learning, mathematics, computational biology, or a related field

- **Strong publication record** in top-tier venues (e.g., NeurIPS, ICML, ICLR, JMLR, AAAI)
- **Experience with modern deep learning frameworks** (e.g., PyTorch, JAX, TensorFlow)
- **Background in at least one of the following:** graph learning, scientific computing, surrogate modeling, or ML theory
- **Interest in interdisciplinary research and real-world scientific problems** (e.g., biology, medicine, chemistry, physics)

We Offer

- A **dynamic and collaborative research environment** across AI and the life sciences
- Access to **compute infrastructure**, and **expert collaborators**
- **Flexibility** to shape your own research agenda within the project themes
- **Close mentorship** from leading researchers in geometric deep learning
- **Competitive salary and benefits**, an employment contract for 3+ years

Application Details

Please apply online and submit the following material and information:

- Curriculum vitae (including a full publication list)
- A short research statement (1–2 pages) explaining your interests and fit for the position
- Names and contact information for two references

The application deadline is 31.8.2025.

We will immediately start to review applications until the position is filled.

We strongly encourage applications from individuals of all backgrounds, especially those traditionally underrepresented in AI and scientific research.

Living and Working in Vienna

Vienna is a truly international city that blends a rich cultural heritage with a modern, vibrant atmosphere. Renowned for its world-class music, art, and culinary scenes, it also offers exceptional public infrastructure, top-quality healthcare, and a safe environment, and is consistently ranked as one of the most livable in the world. As a global scientific hub, Vienna hosts numerous research institutions

and fosters a collaborative, multicultural community that welcomes scientists from around the world.

<https://www.eiu.com/n/campaigns/global-liveability-index-2024/>

AITHYRA is an inclusive employer. We value diversity and strongly encourage applications from all qualified individuals, regardless of background, race, gender, or personal identity.

Learn more about the institute: <https://www.oeaw.ac.at/aithyra>

Also add us at [LinkedIn](#) or [BlueSky](#)!

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